Abstract Submitted
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DFT calculation of Landau levels in 2D crystals: from black phosphorus to dichalcogenides[1] JOSE LADO, JOAQUIN FERNANDEZ ROSSIER, International Iberian Nanotechnology Laboratory — We present a method to calculate the Landau levels and the corresponding edge states of two dimensional (2D) crystals using as a starting point their electronic structure as obtained from standard density functional theory (DFT). The DFT Hamiltonian is represented in the basis of maximally localized Wannier functions [1]. This defines a tight-binding Hamiltonian for the bulk that can be readily used to describe other structures, such as ribbons, provided that atomic scale details of the edges are ignored. The effect of the orbital magnetic field is described using the Peierls substitution. By implementing this approach in a ribbon geometry we recover known results for graphene, MoS_2 [2] and black phosphorous [3]. We apply this method to predict the Landau level spectrum of MoSSe. Our procedure can readily be used in any other 2D crystal, and provides an alternative to effective mass descriptions. [1] A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt and N. Marzari Comput. Phys. Commun. 178, 685 (2008) [2] Habib Rostami and Reza Asgari, Phys. Rev. B 91, 075433 (2015) [3] J. M. Pereira, Jr. and M. I. Katsnelson, Phys. Rev. B 92, 075437 (2015)

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Jose Lado
International Iberian Nanotechnology Laboratory

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